

# Inclusion of phonon exchange in a nuclear matrix element

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## Abstract

Phonon exchange with nuclei in the course of fusion reactions that occur in a solid have not been analyzed previously. This problem has become of interest in connection with claims of observations of anomalies in metal deuterides. If the strong force interaction were dependent only on position (and not spin or isospin), then the coupling with phonons can be developed directly. Since a nuclear interaction can change the lattice constituents, the initial and final state lattices can be different, and we must include this in the formulation. For more realistic strong force models with spin and isospin dependence, we can use correlated nuclear wavefunctions which are made up of products of space, spin and isospin components. In this case, the spin and isospin algebra can be done analytically, producing channel-dependent potentials that are only space dependent. The formulation that results can be used for quantitative estimates of phonon exchange.

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## I. INTRODUCTION

Few claims have resulted in as much controversy as the claim of the observation of an excess heat effect of nuclear origin in metal deuterides made by Fleischmann, Pons, and Hawkins in 1989.<sup>1</sup> Reviews of work on this problem were conducted by the Department of Energy (in the United States) in 1989<sup>2</sup> and in 2004.<sup>3</sup> The conclusions of the 1989 review were very negative. The 2004 review was quite different in how it was carried out, what material was reviewed, and in the results. On the specific question of the existence of an excess power effect, which was the central issue of the review material presented to DoE,<sup>4</sup> there were more positive comments than negative comments volunteered from the reviewers.<sup>5</sup> This is significant, as DoE did not charge the reviewers to consider this question specifically. Among many other comments that were made, several of the reviewers suggested that more work on this problem be submitted to mainstream journals.

Our interest in this paper is not focused on the question of the existence of an excess heat effect, although this issue has motivated our investigations. We are interested instead in theoretical issues which must be better understood in order for theory to be more relevant to the problem. For most physicists, the theoretical problem was adequately addressed by Huizenga, who argued that three “miracles” were required for a theoretical explanation.<sup>6</sup>

- The first “miracle” involves the question of reaction rate. The excess heat effect implies reaction rates on the order of  $10^{12} \text{ sec}^{-1}$ , tens of orders of magnitude larger than the fastest fusion rates possible in molecular  $\text{D}_2$  or  $\text{HD}$ .
- The second “miracle” concerns the branching ratio. Fleischmann initially speculated that  $^4\text{He}$  was being made from two deuterons. Such a result is seemingly miraculous as the branching ratio for this reaction channel is lower by about seven orders of magnitude than the primary  $\text{n}+^3\text{He}$  and  $\text{p}+\text{t}$  reaction channels.
- The third “miracle” involves the requirement that the reaction energy be expressed through channels not involving energetic reaction products.

If one believes that these issues are insurmountable, then one would require that any claim of excess heat of nuclear origin must be accompanied by measurable energetic reaction products. This view was adopted by Huizenga, and by the 1989 ERAB Panel. This view is also widely held among the physics community at this time.

### A. Motivation

However, other views are possible. Fleischmann’s initial speculation was that a new physical process was involved, one that behaves differently from what is described in the textbooks. It seems that if we are trying to understand whether an excess heat effect

can exist, we should be asking whether there can be interactions between nuclei and a condensed matter environment. For example, suppose that phonons are exchanged in the course of a nuclear reaction that occurs in a lattice. Could this phonon exchange result in a modification of the selection rules? And if phonon exchange occurs, would that not constitute a new channel into which reaction energy might go? Nuclear physics relies heavily on the notion of an equivalent vacuum reaction in order to understand quantitatively fusion reactions. Huizenga’s three “miracles” reflect such a view. For example, the second “miracle” is essentially a statement of energy, linear momentum, and angular momentum conservation, all of which are conserved in vacuum. Is it obvious that conservation laws in a condensed matter environment always produce the same reaction pathways with the same branching ratios; and, if so, can this be proven? In the case of the third “miracle,” the reaction energy must be expressed as an energetic product in vacuum, since no other kinds of channels exist. But is it obvious that this must also be the case in a condensed matter environment, where low energy channels do exist? Once again, can this be proven? In any event, all of these questions ought to be capable of being addressed by theory.

The current lack of such a theory in the mainstream literature is underscored in comments made by some reviewers in the 2004 DoE review. For example, a reviewer with expertise in metal deuterides and phonons wrote: “To create a coupling between nuclear interaction and phonons at such a low energy region (namely, the electromagnetic interaction) is beyond one’s imagination at the moment.” Another reviewer with expertise in nuclear theory wrote: “I am convinced that simple order-of-magnitude estimates of this kind could quickly rule out any of the exotic mechanisms proposed...” This reviewer argues that the matrix element for the emission of a large number of phonons would scale as  $(kR)^{2L}$ , where  $k$  is the phonon wavenumber. Aside from the fact that the emission of a large number of phonons in a single process was not put forth as a proposed reaction mechanism in the review, the use (or misuse) by this reviewer of a phonon wavenumber in this way underscores the need for a relevant theory. We find ourselves then in a position where a better understanding of phonon exchange in fusion reactions is required for a sensible discussion of these and related issues. This motivates us to consider in this manuscript how to calculate phonon exchange in perhaps the simplest application; that of an interaction matrix element. Phonon exchange due to recoil in neutron capture reactions was analyzed by Lamb,<sup>7</sup> and this analysis has been used subsequently for phonon exchange in gamma reactions. In the Mössbauer effect, an anomalous zero-phonon exchange effect occurs if the recoil is sufficiently gentle.<sup>8</sup> In our matrix elements recoil is involved implicitly, and phonon exchange due to the local change in lattice structure will appear explicitly.

## B. Excitation transfer scheme

In the following sections of this manuscript, we develop a formulation suitable for including phonon exchange in nuclear reaction matrix elements. Once armed with this tool, we are in a position to develop calculations relevant to candidate reaction schemes that involve phonon exchange (of which quite a few have been proposed over the years). Our current interest is focused on a particular scheme in which coupling occurs between nuclei at different sites as a result of phonon exchange with a common phonon mode. In this scheme, two deuterons fuse locally with the reaction energy transferred elsewhere through a second-order off-resonant excitation transfer effect. The systematics of this effect in the idealized case of two-level systems coupled to a common oscillator is discussed in a recent analysis.<sup>9</sup> In essence, the reaction energy is transferred to excited states in host lattice nuclei through an initial slow excitation transfer step, and then subsequent rapid excitation transfer occurs among these nuclei. The reaction energy is transferred to the phonon mode in this scheme a few phonons at a time in a very large number of fast excitation transfer reactions. The scheme seems to be closely related to experiment, and the reaction rate predicted appears to be consistent with experiment to within uncertainties in the deuteron-deuteron screening. The evaluation of this scheme requires the ability to evaluate phonon exchange in fusion reactions as discussed in the present manuscript.

Huizenga's arguments are based ultimately on fundamental notions relevant to vacuum reactions, local energy and momentum conservation, and the use of Golden Rule reaction rate estimates, as discussed above. In this new excitation transfer scheme, the energy of the coupled system is conserved, but local energy is transferred elsewhere. In addition, the associated reaction dynamics do not follow simple Golden Rule predictions. Huizenga's arguments simply do not apply to this kind of scheme.

## C. Overview of the paper

This paper is organized as follows. In section II we discuss the basic lattice-nuclear coupling (assuming a simplified nuclear potential model that depends only on position), and argue that it is very similar to the more familiar electron-phonon and neutron-phonon couplings. However, realistic nuclear potentials depend on spin, isospin, and parity. In Section III we show that for realistic nuclear potentials, by first doing the spin and isospin algebra analytically, the ideas developed in Section II are relevant. In Section IV, using the Hamada-Johnston nuclear potential, we explicitly carry out the program outlined in Section III for one particular matrix element relevant to a deuteron-deuteron fusion reaction. This particular interaction is chosen because it is one of the simplest realistic nuclear potentials. In Section V we extend this vacuum result to include the lattice. We find in Section VI an explicit expression for one of the integrals that appears in the interaction matrix element in

terms of phonon coordinates. This result is closely related to the discussion in Section II. A summary and conclusions is given in Section VII.

Although the essential issues involved in phonon exchange can be seen with the simplified position-dependent potential, we need to work with nuclear wavefunctions that depend on spin and isospin when using a more realistic nuclear potential model. The construction of these general four-body correlated nuclear wavefunction requires the use of certain aspects of representation theory, and may be unfamiliar to some of the readers. As a result, we have included material in a set of appendices that provide further discussion of the wavefunction construction and usage in matrix element calculations.

## II. PHONON INTERACTIONS

We are interested in the basic issue of phonon exchange in association with nuclear reactions in a lattice. The formulation that follows in subsequent sections is complicated, and it makes sense to review phonon exchange in more familiar circumstances. In condensed matter physics, phonon exchange is of interest in the study of electron scattering and neutron scattering. In both cases, phonon exchange comes about through a formulation in which the center of mass coordinates of the nuclei are taken to be phonon operators.

### A. Phonon exchange associated with electronic transitions

For example, electron-phonon interactions can be developed ultimately starting from the Coulomb interaction written in the form<sup>10</sup>

$$- \sum_{j,k} \frac{Z_j e^2}{|\hat{\mathbf{R}}_j - \mathbf{x}_k|} \quad (1)$$

where the  $\mathbf{x}_k$  are the electron coordinates, and the  $Z_j$  are the effective charges on the ions. The  $\hat{\mathbf{R}}_j$  are the nuclear center of mass coordinates, which are dynamical, and which we think of in terms of lattice operators ( $\hat{q}_m$ )

$$\hat{\mathbf{R}}_j = \mathbf{R}_j(\hat{q}_1, \hat{q}_2, \dots) \quad (2)$$

In the event that we adopt a description of the lattice in terms of product states, then a matrix element of the Coulomb interaction might be written as

$$M_{fi} = - \left\langle \Psi_f^L(\{q\}) \psi_f(\{\mathbf{x}\}) \left| \sum_{j,k} \frac{Z_j e^2}{|\hat{\mathbf{R}}_j - \mathbf{x}_k|} \right| \Psi_i^L(\{q\}) \psi_i(\{\mathbf{x}\}) \right\rangle \quad (3)$$

In this way of thinking about the problem, we could define a phonon interaction by integrating over electronic coordinates

$$\hat{v}_{fi}(\{q\}) = - \left\langle \psi_f(\{\mathbf{x}\}) \left| \sum_{j,k} \frac{Z_j e^2}{|\hat{\mathbf{R}}_j - \mathbf{x}_k|} \right| \psi_i(\{\mathbf{x}\}) \right\rangle \quad (4)$$

Phonon exchange in this case can be developed then from lattice matrix elements of this operator

$$M_{fi} = \langle \Psi_f^L(\{q\}) | \hat{v}_{fi}(\{q\}) | \Psi_i^L(\{q\}) \rangle \quad (5)$$

In the event that the electronic transition results in a change in the local force constants, the initial and final state lattice may differ enough that this should be reflected in the matrix element.

## B. Phonon exchange associated with neutron interactions

A similar approach can be used in the case of neutron scattering. In the case of a simple position-dependent interaction

$$V_0 \sum_j \delta^3(\hat{\mathbf{R}}_j - \mathbf{r}_n) \quad (6)$$

we can develop the phonon interaction according to

$$\hat{v}_{fi}(\{q\}) = \left\langle \psi_f(\mathbf{r}_n) \left| V_0 \sum_j \delta^3(\hat{\mathbf{R}}_j - \mathbf{r}_n) \right| \psi_i(\mathbf{r}_n) \right\rangle \quad (7)$$

In these equations  $\mathbf{r}_n$  is the neutron coordinate. With a knowledge of the phonon interaction, we can analyze phonon exchange using  $M_{fi}$  matrix elements as calculated above.

## C. Phonon exchange in a simplified model for nuclear reactions

We might choose to work with an approximate position-dependent nuclear interaction model that is a function of spatial coordinates alone

$$\sum_{\alpha < \beta} v_n(|\mathbf{r}_\alpha - \mathbf{r}_\beta|) \quad (8)$$

where  $\alpha$  and  $\beta$  refer to nucleon (neutron and proton) coordinates. The interaction matrix element in this case can be written as

$$M_{fi} = \left\langle \Psi_f^L(\{\mathbf{r}\}) \left| \sum_{\alpha < \beta} v_n(|\mathbf{r}_\alpha - \mathbf{r}_\beta|) \right| \Psi_i^L(\{\mathbf{r}\}) \right\rangle \quad (9)$$

where the integration here is taken over individual nucleon coordinates. A nuclear reaction may result in the initial lattice being different than the final lattice. For example, if two deuterons reacted to form  ${}^3\text{He} + n$ , the initial lattice would contain the two deuterons while the final lattice would have  ${}^3\text{He}$  and a possibly free neutron. We note that in a normal version of this reaction, the final state products would fly off as energetic nuclear products; we consider this possibility to be included within the formulation under discussion.

However, this description does not yet make clear the situation with respect to phonon exchange. For this, we need to rewrite the integral in terms of phonon coordinates rather than in terms of nucleon coordinates. To make progress, we can express individual nucleon coordinates that are associated with nuclei in terms of the nuclear center of mass coordinates  $\mathbf{R}$  and relative internal nuclear coordinates  $\boldsymbol{\xi}$

$$\Psi^L(\{\mathbf{r}\}) = \Psi^L(\{\mathbf{R}\}, \{\boldsymbol{\xi}\}) \quad (10)$$

Since a nuclear reaction may result in a change in nuclei between the initial states and the final states, the set of center of mass coordinates may be different. Consequently, the nuclear interaction matrix element can be written formally as

$$M_{fi} = \int \left[ \Psi_f^L(\{\mathbf{R}^f\}, \{\boldsymbol{\xi}^f\}) \right]^* \sum_{\alpha < \beta} v_n(|\mathbf{r}_\alpha - \mathbf{r}_\beta|) \Psi_i^L(\{\mathbf{R}^i\}, \{\boldsymbol{\xi}^i\}) \prod_{\alpha} \delta^3(\mathbf{r}_\alpha^i - \mathbf{r}_\alpha^f) d\{\boldsymbol{\xi}^i\} d\{\boldsymbol{\xi}^f\} d\{\mathbf{R}^i\} d\{\mathbf{R}^f\} \quad (11)$$

We integrate over all initial and final state center of mass and internal coordinates, and require that the individual nucleon coordinates be the same in the initial and final states.

Once we have a description in terms of the nuclear center of mass coordinates, we can rewrite the integrations in terms of phonon coordinates. To simplify things, we might assume product states of the form

$$\Psi^L(\{\mathbf{R}\}, \{\boldsymbol{\xi}\}) \rightarrow \Psi^L(\{q\})\Phi(\{\boldsymbol{\xi}\}) \quad (12)$$

In this case, the matrix element becomes

$$M_{fi} = \int \left[ \Psi_f^L(\{q^f\})\Phi_f(\{\boldsymbol{\xi}^f\}) \right]^* \sum_{\alpha < \beta} v_n(|\mathbf{r}_\alpha - \mathbf{r}_\beta|) \Psi_i^L(\{q^i\})\Phi_i(\{\boldsymbol{\xi}^i\}) \prod_{\alpha} \delta^3(\mathbf{r}_\alpha^i - \mathbf{r}_\alpha^f) d\{\boldsymbol{\xi}^i\} d\{\boldsymbol{\xi}^f\} d\{q^i\} d\{q^f\} \quad (13)$$

For a final lattice with  $N$  ions, this can be thought of as

$$M_{fi} = \int \left[ \Psi_f^L(\mathbf{q}^f) \right]^* \hat{v}_{fi}(\mathbf{q}^f, \mathbf{q}^i) \Psi_i^L(\mathbf{q}^i) \delta^{(3N-3)}(\mathbf{q}^f - \mathbf{A} \cdot \mathbf{q}^i - \mathbf{b}) d\mathbf{q}^i d\mathbf{q}^f \quad (14)$$

in which the phonon interaction operator  $\hat{v}_{fi}(\mathbf{q}^f, \mathbf{q}^i)$  is developed from an appropriate integration over the internal nuclear coordinates. More simply, we may write

$$M_{fi} = \int \left[ \Psi_f^L(\mathbf{q}^f) \right]^* \hat{v}_{fi}(\mathbf{q}^f, \mathbf{q}^i) \Psi_i^L(\mathbf{q}^i) d\mathbf{q}^i \quad (15)$$

together with the associated constraint

$$\mathbf{q}^f = \mathbf{A} \cdot \mathbf{q}^i + \mathbf{b} \quad (16)$$

Due to the change in the lattice structure, the phonon mode structure can be altered.<sup>11,12</sup> The associated matrix element written in terms of initial state and final state coordinates [equation (15)] is common in papers on Franck-Condon factors in polyatomic molecules.<sup>13</sup>



## D. Discussion

Phonon exchange in electron and neutron scattering can be implemented using the local nuclear center of mass operators as phonon operators. This leads to a straightforward description of matrix elements that include phonon exchange, as well as the development of phonon exchange operators. In the case of a nuclear reaction, we can define a nuclear interaction matrix element simply enough under the assumption of a position-dependent potential as long as we work with nucleon coordinates. However, when the integral is rewritten in terms of phonon mode amplitudes, the resulting expression is more complicated. The underlying ideas and approach are very similar. The important message here is that a nuclear interaction matrix element expressed in terms of the nucleons of the lattice is completely straightforward, and it is only the bookkeeping associated with the assembly of nucleons into nuclei, and nuclei into phonons, that adds some complication to the problem.

There are basic differences between the new problem and the well known electron and neutron scattering problems which deserve to be noted.

- The energy scales in the case of nuclear reactions are not matched; typical nuclear reaction energies are on MeV scale, whereas the maximum phonon energies are typically 100 meV or less.
- A nuclear reaction involving a change in the nucleon content of the product nuclei will likely produce phonon exchange, if for no other reason than the fact that such reactions will produce a change in the structure of the lattice.

### III. FORMAL CALCULATION WITH A REALISTIC POTENTIAL

For quantitative results, we will need to use a realistic nuclear potential. In atomic physics and solid state physics, we are familiar with wavefunctions that have both spin and space dependence. Nuclear wavefunctions have in addition isospin dependence. In the isospin scheme, a nucleon can be in an isospin down state  $|\downarrow\rangle$  in which case it is a neutron, or it can be in an isospin up state  $|\uparrow\rangle$  in which case it is a proton. It was recognized early on in nuclear physics that the nucleon-nucleon potential is of short range in space, and depends explicitly on both spin and isospin. Over the past 60 years, increasingly accurate nuclear potential models have been developed. Early models were based in part on field theoretical models for the one-pion exchange, and in part on few parameter empirical models that were fit to scattering data. In recent years, the most accurate nuclear potential models have been constructed from a diagrammatic analysis of an effective field theory.<sup>14,15</sup> For the purposes of the present paper, we will adopt an early potential model (the Hamada-Johnston potential<sup>16</sup>), which has the advantage for our discussion of being relatively simple in form.

#### A. Hamada-Johnston potential

The Hamada-Johnston potential between nucleon 1 and nucleon 2 appears in the literature written as

$$V_{HJ}(1,2) = V_C(1,2) + V_T(1,2)S_{12} + V_{LS}(1,2)(\mathbf{L}\cdot\mathbf{S}) + V_{LL}(1,2)L_{12} \quad (17)$$

This potential is made up of four basic terms: a central potential  $V_C$ ; a tensor interaction  $V_T S_{12}$ ; a spin-orbit term  $V_{LS}(\mathbf{L}\cdot\mathbf{S})$ ; and a generalized centripetal potential term  $V_{LL} L_{12}$ . These are discussed further in Appendix A. The central and tensor terms have isospin dependence, whereas the spin-orbit and generalized centripetal terms do not. As an example, we consider the tensor term in more detail (which we use as an example in Appendix D). Explicitly it is given by

$$V_T(1,2)S_{12} = (\boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2) y_T(\mu r_{12}) \left[ 3 \frac{(\boldsymbol{\sigma}_1 \cdot \mathbf{r}_{12})(\boldsymbol{\sigma}_2 \cdot \mathbf{r}_{12})}{r_{12}^2} - \boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2 \right] \quad (18)$$

with  $\mu = m_\pi c/\hbar$ , where  $m_\pi$  is the mass of the pion. The radial potential is parameterized according to

$$y_T(x) = 0.08 \frac{m_\pi c^2}{3} \left( 1 + \frac{3}{x} + \frac{3}{x^2} \right) \frac{e^{-x}}{x} \left[ 1 + a_T \frac{e^{-x}}{x} + b_T \frac{e^{-2x}}{x^2} \right] \quad (19)$$

where  $a_T$  and  $b_T$  are parameters which have been fit separately for singlet-triplet spin and even-odd parity (angular momentum) channels. Hence,  $y_T$  has an additional implicit dependence on spin and parity:  $y_T = y_T^\alpha$  where  $\alpha$  can be even-triplet (*et*), even-singlet (*es*), odd-triplet(*ot*) or odd-singlet(*os*).

## B. Wavefunctions

Because realistic nuclear potentials have explicit dependences on spin and isospin, one requires nuclear wavefunctions that have well defined spin and isospin dependences. In the nuclear physics literature, there are a variety of approaches to this problem, ranging from determinantal wavefunctions built up from single nucleon orbitals to more complicated correlated wavefunctions. For the development of the results in this paper, we will adopt a basic construction of correlated wavefunctions in terms of products of spatial, spin-dependent, and isospin-dependent pieces, each of which is determined by group theory.

As is customary in nuclear physics, we choose our wavefunctions to satisfy the generalized Pauli exclusion principle, which requires that the total wavefunction (including space, spin and isospin parts) has to be antisymmetric with respect to nucleon exchange. A group theoretical construction of the antisymmetric wavefunctions is possible by summing over products of many-particle spatial functions, spin functions, and isospin functions, each of which belong to appropriate representations of the symmetric group,  $S(4)$ .<sup>17</sup> In the case of the spin and isospin functions, the symmetric group representations correspond to eigenfunctions of total spin and isospin, as a consequence of the Schur-Weyl duality.<sup>18,19</sup> Hence the antisymmetric wavefunctions have well-defined total spin and isospin. This is discussed in Appendix B.

In general, such correlated wavefunctions can be written in the form

$$\Psi = \sum_j C_j s_j(\{\sigma\}) t_j(\{\tau\}) \psi_j(\{\mathbf{r}\}) \quad (20)$$

where  $s_j(\{\sigma\})$  are the spin functions,  $t_j(\{\tau\})$  are the isospin functions, and  $\psi_j(\{\mathbf{r}\})$  are the spatial functions; all of which belong to certain representations of the symmetric group as indicated above. The  $C_j$  are products of the Clebsch-Gordan coefficients of  $S(4)$ .

## C. Formal matrix element calculation

Given the discussion above, the basic calculation of an interaction matrix element is straightforward. We begin with initial and final states defined as

$$\Psi = \sum_j C_j s_j(\{\sigma\}) t_j(\{\tau\}) \psi_j(\{\mathbf{r}\}) \quad \Psi' = \sum_k C_k s'_k(\{\sigma\}) t'_k(\{\tau\}) \psi'_k(\{\mathbf{r}\}) \quad (21)$$

We then formally calculate the matrix element to give

$$\begin{aligned}
\left\langle \Psi \left| \sum_{\alpha < \beta} V_{HJ}(\alpha, \beta) \right| \Psi' \right\rangle &= \\
\left\langle \sum_j C_j s_j(\{\sigma\}) t_j(\{\tau\}) \psi_j(\{\mathbf{r}\}) \left| \sum_{\alpha < \beta} V_{HJ}(\alpha, \beta) \right| \sum_k C_k s'_k(\{\sigma\}) t'_k(\{\tau\}) \psi'_k(\{\mathbf{r}\}) \right\rangle \\
&= \sum_{j,k} \left\langle \psi_j(\{\mathbf{r}\}) \left| V_R^{j,k}(\{\mathbf{r}\}) \right| \psi'_k(\{\mathbf{r}\}) \right\rangle
\end{aligned} \tag{22}$$

In writing this, we have integrated formally over spin and isospin coordinates to develop the interaction matrix element into simpler spatial matrix elements involving individually position-dependent potentials  $V_R^{j,k}$  given by

$$V_R^{j,k}(\{\mathbf{r}\}) = C_j^* C_k \left\langle s_j(\{\sigma\}) t_j(\{\tau\}) \left| \sum_{\alpha < \beta} V_{HJ}(\alpha, \beta) \right| s'_k(\{\sigma\}) t'_k(\{\tau\}) \right\rangle \tag{23}$$

In this way we can reduce the spin and isospin dependent nuclear matrix element into a set of simpler matrix elements, each one of which involves a position-dependent potential.

## IV. BASIC VACUUM MATRIX ELEMENT CALCULATION

Before attempting a calculation of a specific interaction matrix element in the lattice case, it is appropriate to first examine the simpler equivalent calculation in the vacuum case. For this specific calculation, we will select a four-body problem in which there are two deuterons in the initial state, and in which the final state contains a three nucleon body ( ${}^3\text{He}$  or  $t$ ) and a one nucleon body ( $n$  or  $p$ ).

### A. Vacuum nuclear wavefunctions

The specific matrix element that we select for our example involves a quintet ( $S = 2, M_S = 1$ ) initial state  $\Psi_i$  with two deuterons (the deuterons each have spin 1), and a singlet ( $S = 0, M_S = 0$ ) final state which is a linear combination of  ${}^3\text{H} + p$  and  ${}^3\text{He} + n$ . The reason for this is that a linear combination of states with different total isospin ( $T = 0$  and  $T = 1$ ) are required to resolve a single proton or neutron in the final state channel. For simplicity, we have adopted initial and final state wavefunctions with total isospin  $T = 0$ . As we discussed briefly above, nuclear wavefunctions can be constructed from linear combinations of products of basis vectors of representations of the symmetric group. For the case of four-body wavefunctions, we have indexed the specific basis vectors in terms of their associated Yamanouchi symbol in Appendix B. We have also listed the results of a systematic construction of all such four-body wavefunctions with total isospin zero in Appendix C.

The initial state is constructed according to

$$\Psi_i = \Psi_6 = \frac{1}{\sqrt{2}} [\psi_5 s_{10} t_6 - \psi_6 s_{10} t_5] \quad (24)$$

where  $\Psi_6$  is the notation used in systematic construction of Appendix B. Each of the four-particle spin ( $s$ ), isospin ( $t$ ), and spatial ( $\psi$ ) functions are individually basis vectors of representations of the symmetric group listed in Appendix B. The final state is constructed according to

$$\Psi_f = \Psi_1 = \psi_{10} \frac{1}{\sqrt{2}} [s_5 t_6 - s_6 t_5] \quad (25)$$

where  $\Psi_1$  is also the notation used in Appendix B. We have selected these states in particular due to the close correspondence between the physical states discussed below, and the group theoretical Yamanouchi basis states for these channels. In the case of other channels, a linear superposition of Yamanouchi basis states may be required.

## B. Matrix element in terms of Yamanouchi basis functions

The matrix element can be evaluated using the approach discussed above. We first express the matrix elements in terms of  $V_{HJ}(1, 2)$ , since the Yamanouchi basis functions are either symmetric or antisymmetric under  $1 \leftrightarrow 2$ . We write

$$\left\langle \Psi_f \left| \sum_{\alpha < \beta} V_{HJ}(\alpha, \beta) \right| \Psi_i \right\rangle = 6 \langle \Psi_f | V_{HJ}(1, 2) | \Psi_i \rangle \quad (26)$$

Using the initial and final states in the form listed above, we obtain four different contributions to the matrix element

$$\begin{aligned} M_{fi} = 3 \bigg[ & \langle s_5 t_6 \psi_{10} | V_{HJ}(1, 2) | s_{10} t_6 \psi_5 \rangle - \langle s_5 t_6 \psi_{10} | V_{HJ}(1, 2) | s_{10} t_5 \psi_6 \rangle \\ & - \langle s_6 t_5 \psi_{10} | V_{HJ}(1, 2) | s_{10} t_6 \psi_5 \rangle + \langle s_6 t_5 \psi_{10} | V_{HJ}(1, 2) | s_{10} t_5 \psi_6 \rangle \bigg] \quad (27) \end{aligned}$$

Because of the symmetry of the interaction and the wavefunctions, only one term survives the spin and isospin algebra. The details of this calculation for the tensor term are worked out in Appendix D. The generalized centripetal term can be worked out in a completely analogous way. The net result is that

$$M_{fi} = \langle \psi_{10} | V_R^{10,5}(1, 2) | \psi_5 \rangle \quad (28)$$

where

$$V_R^{10,5}(1, 2) = 18\sqrt{3} \frac{(x_{12} + iy_{12}) z_{12}}{r_{12}^2} y_T^{et}(\mu r_{12}) + \frac{\sqrt{3}}{\hbar^2} (\hat{L}_+ \hat{L}_z + \hat{L}_z \hat{L}_+) y_{LL}^{et}(\mu r_{12}) \quad (29)$$

where  $\hat{L}_z$  and  $\hat{L}_+$  are relative 12 (read as one-two) angular momentum operators.

We have already noted that the Yamanouchi basis is naturally purely symmetric or antisymmetric under the exchange  $1 \leftrightarrow 2$  (This is further discussed in Appendix D). As a consequence, the calculation of the many-body matrix element leads to the simplest algebraic result when specified in terms of 12 terms. Interactions between all particles are represented, since the  $\psi_{10}$  and  $\psi_5$  representations include permutations of the particle numbering. Hence, the use of a position-dependent interaction potential given in terms of  $\mathbf{r}_{12}$  is appropriate, and implies the use of  $\mathbf{r}_{12}$  as a favored relative coordinate to use in the evaluation of the spatial matrix element.

### C. Physical wavefunctions

The group theoretical machinery that we used in the evaluation above results in a compact expression given in terms of spatial Yamanouchi basis functions. As such, they have certain symmetries with respect to particle interchange. These must be implemented in the construction of the spatial wavefunctions. This can be accomplished by using an appropriate superposition of permutations of wavefunctions with no particular symmetry.

For example, suppose we begin with an unsymmetrized “physical” wavefunction for the two deuteron initial state

$$\psi(12; 34) = \phi_d(\mathbf{r}_2 - \mathbf{r}_1) \phi_d(\mathbf{r}_4 - \mathbf{r}_3) F_{2,2} \left( \frac{\mathbf{r}_1 + \mathbf{r}_2}{2}, \frac{\mathbf{r}_3 + \mathbf{r}_4}{2} \right) \quad (30)$$

In this wavefunction, nucleons 1 and 2 make up one deuteron given by  $\phi_d(\mathbf{r}_2 - \mathbf{r}_1)$ , and nucleons 3 and 4 make up another deuteron  $\phi_d(\mathbf{r}_4 - \mathbf{r}_3)$ . The generalized channel separation function  $F_{2,2}$  is the probability amplitude associated with the two center of mass coordinates of the deuterons. As discussed in Appendix E, we can use this unsymmetrized physical wavefunction as the basis for the construction of the associated Yamanouchi  $\psi_5$  function, which leads to

$$\psi_5 = \frac{1}{\sqrt{12}} \left[ 2\psi(12; 34) + 2\psi(34; 21) - \psi(23; 14) - \psi(14; 23) - \psi(13; 24) - \psi(24; 13) \right] \quad (31)$$

This generates the appropriate Yamanouchi basis vector for use in the matrix element expression above.

In the case of the final state channel, we begin with the physical wavefunction

$$\psi(123; 4) = \phi_{3He}(\mathbf{r}_3 - \mathbf{r}_2, \mathbf{r}_2 - \mathbf{r}_1) F_{3,1} \left( \frac{\mathbf{r}_1 + \mathbf{r}_2 + \mathbf{r}_3}{3}, \mathbf{r}_4 \right) \quad (32)$$

where  $\phi_{3He}$  is the  $^3\text{He}$  wavefunction specified in terms of two relative internal coordinates, and where  $F_{3,1}$  is the generalized channel function for the center of mass for the  $^3\text{He}$  and neutron. From this physical wavefunction, we can construct the associated Yamanouchi  $\psi_{10}$  function according to

$$\psi_{10} = \frac{1}{2} \left[ \psi(123; 4) + \psi(124; 3) + \psi(134; 2) + \psi(234; 1) \right] \quad (33)$$

This function can be used in the group theoretical matrix element formula above.

## V. LATTICE RESULT

Let us now consider exactly the same physical process taking place inside the lattice. We are interested in the calculation of the interaction matrix element with wavefunctions that contain both nuclear and lattice coordinates. Perhaps the simplest way to approach the problem is to make use of the vacuum results from the last section, but expand the definition of the initial and final states to include the lattice.

### A. Wavefunctions for lattice and nuclei

We now augment the definition of the physical wavefunctions to include the lattice coordinates. For example, in the new physical initial state wavefunction, we include the center of mass coordinates of the other nuclei to obtain

$$\psi(12; 34, \{\mathbf{R}\}) = \phi_d(\mathbf{r}_2 - \mathbf{r}_1) \phi_d(\mathbf{r}_4 - \mathbf{r}_3) F_{2,2}^L \left( \frac{\mathbf{r}_1 + \mathbf{r}_2}{2}, \frac{\mathbf{r}_3 + \mathbf{r}_4}{2}, \{\mathbf{R}\} \right) \quad (34)$$

The other nuclei in the lattice are spectators in the sense that they do not participate in nucleon rearrangement associated with the reaction. Consequently, the appearance of the associated degrees of freedom into the lattice channel separation factor is an appropriate generalization of the generalized channel separation factor from the vacuum case. We still require the nucleons that participate in the reaction to be described by a wavefunction that is totally antisymmetric under the exchange of nucleons. The vacuum formulation that we discussed above accomplished this in the absence of spectator nuclei. There seems to be no reason that we cannot adopt precisely the same kind of formulation here (this is discussed in Appendix F). Hence, we form the appropriate Yamanouchi spatial basis function for the initial state made up of the same superposition of physical states that are augmented with spectator coordinates. This leads to

$$\begin{aligned} \psi_5^L = \frac{1}{\sqrt{12}} & \left[ 2\psi(12; 34, \{\mathbf{R}\}) + 2\psi(34; 21, \{\mathbf{R}\}) - \psi(23; 14, \{\mathbf{R}\}) \right. \\ & \left. - \psi(14; 23, \{\mathbf{R}\}) - \psi(13; 24, \{\mathbf{R}\}) - \psi(24; 13, \{\mathbf{R}\}) \right] \end{aligned} \quad (35)$$

Final state wavefunctions can be developed similarly. The physical wavefunction for the final state is

$$\psi(123; 4, \{\mathbf{R}\}) = \phi_{3He}(\mathbf{r}_3 - \mathbf{r}_2, \mathbf{r}_2 - \mathbf{r}_1) F_{3,1}^L \left( \frac{\mathbf{r}_1 + \mathbf{r}_2 + \mathbf{r}_3}{3}, \mathbf{r}_4, \{\mathbf{R}\} \right) \quad (36)$$

The appropriate final state Yamanouchi basis is formed through



$$\psi_{10}^L = \frac{1}{2} \left[ \psi(123; 4, \{\mathbf{R}\}) + \psi(124; 3, \{\mathbf{R}\}) + \psi(134; 2, \{\mathbf{R}\}) + \psi(234; 1, \{\mathbf{R}\}) \right] \quad (37)$$

### B. Matrix element

We can take advantage of the same group theoretical construction to evaluate the matrix element when spectator nuclei are present, since we only required total antisymmetrization on the four nucleons involved in the local strong force interaction. Consequently, we may write

$$M_{fi} = \langle \psi_{10}^L | V_R^{10,5} | \psi_5^L \rangle \quad (38)$$

We see in this result a very strong connection between the vacuum result and the lattice result. In general we can systematically extend vacuum calculations to the lattice case through the addition of the lattice nuclear center of mass coordinates as spectator degrees of freedom.

### C. Matrix element in terms of physical wavefunctions

We have made use of representations of the symmetric group in order to construct nuclear wavefunctions and to evaluate the interaction matrix element. In the case of the spatial wavefunctions, these basis functions are made up of several different permutations of the physical wavefunction. If we make use of these expansions, we can recast the interaction matrix element in terms of matrix elements involving physical wavefunctions. This will in general produce a large number of terms.

In the specific case of the tensor matrix element that we have been using as an example, we obtain twenty four terms in total. We may write

$$M_{fi} = \frac{1}{\sqrt{12}} \int \left[ \phi_{3He}(\mathbf{r}_3 - \mathbf{r}_2, \mathbf{r}_2 - \mathbf{r}_1) F_{3,1}^L \left( \frac{\mathbf{r}_1 + \mathbf{r}_2 + \mathbf{r}_3}{3}, \mathbf{r}_4, \{\mathbf{R}\} \right) \right]^* V_R^{10,5}(\mathbf{r}_2 - \mathbf{r}_1) \phi_d(\mathbf{r}_2 - \mathbf{r}_1) \phi_d(\mathbf{r}_4 - \mathbf{r}_3) \\ F_{2,2}^L \left( \frac{\mathbf{r}_1 + \mathbf{r}_2}{2}, \frac{\mathbf{r}_3 + \mathbf{r}_4}{2}, \{\mathbf{R}\} \right) d^3\mathbf{r}_1 d^3\mathbf{r}_2 d^3\mathbf{r}_3 d^3\mathbf{r}_4 d^{3N-3}\{\mathbf{R}\} + \dots \quad (39)$$

where the  $\dots$  represent the other twenty three terms in the expansion (see Appendix G).

## VI. MATRIX ELEMENT IN TERMS OF PHONON COORDINATES

A primary goal of this paper is to develop an expression for one of the integrals that appear in the matrix element explicitly in terms of phonon coordinates, similar to what we discussed in Section II. We begin by defining the integral  $I$  according to

$$I = \int \left[ \phi_{3He}(\mathbf{r}_3 - \mathbf{r}_2, \mathbf{r}_2 - \mathbf{r}_1) F_{3,1}^L \left( \frac{\mathbf{r}_1 + \mathbf{r}_2 + \mathbf{r}_3}{3}, \mathbf{r}_4, \{\mathbf{R}\} \right) \right]^* V_R^{10,5}(\mathbf{r}_2 - \mathbf{r}_1) \phi_d(\mathbf{r}_2 - \mathbf{r}_1) \phi_d(\mathbf{r}_4 - \mathbf{r}_3) F_{2,2}^L \left( \frac{\mathbf{r}_1 + \mathbf{r}_2}{2}, \frac{\mathbf{r}_3 + \mathbf{r}_4}{2}, \{\mathbf{R}\} \right) d^3\mathbf{r}_1 d^3\mathbf{r}_2 d^3\mathbf{r}_3 d^3\mathbf{r}_4 d^{3N-3}\{\mathbf{R}\} \quad (40)$$

### A. Integral in terms of center of mass and relative coordinates

This integral includes integrations over nucleon coordinates as well as the center of mass coordinates of the spectator nuclei. We would like to recast the integral in terms of center of mass coordinates and relative coordinates, to set things up for a transformation to phonon mode coordinates. We may write

$$I = \int \left[ \phi_{3He}(\boldsymbol{\xi}_{32}^f, \boldsymbol{\xi}_{21}^f) F_{3,1}^L \left( \mathbf{R}_{3He}^f, \mathbf{r}_4^f, \{\mathbf{R}\} \right) \right]^* V(\boldsymbol{\xi}_{21}^f) \phi_d(\boldsymbol{\xi}_{21}^i) \phi_d(\boldsymbol{\xi}_{43}^i) F_{2,2}^L(\mathbf{R}_{d1}^i, \mathbf{R}_{d2}^i, \{\mathbf{R}\}) \delta^{(3)} \left( -\frac{1}{3}\boldsymbol{\xi}_{32}^f - \frac{2}{3}\boldsymbol{\xi}_{21}^f + \mathbf{R}_{3He}^f - \left( -\frac{1}{2}\boldsymbol{\xi}_{21}^i + \mathbf{R}_{d1}^i \right) \right) \delta^{(3)} \left( -\frac{1}{3}\boldsymbol{\xi}_{32}^f + \frac{1}{3}\boldsymbol{\xi}_{21}^f + \mathbf{R}_{3He}^f - \left( \frac{1}{2}\boldsymbol{\xi}_{21}^i + \mathbf{R}_{d1}^i \right) \right) \delta^{(3)} \left( \frac{2}{3}\boldsymbol{\xi}_{32}^f + \frac{1}{3}\boldsymbol{\xi}_{21}^f + \mathbf{R}_{3He}^f - \left( -\frac{1}{2}\boldsymbol{\xi}_{43}^i + \mathbf{R}_{d2}^i \right) \right) \delta^{(3)} \left( \mathbf{r}_4^f - \left( \frac{1}{2}\boldsymbol{\xi}_{43}^i + \mathbf{R}_{d2}^i \right) \right) d^3\boldsymbol{\xi}_{32}^f d^3\boldsymbol{\xi}_{21}^f d^3\mathbf{R}_{3He}^f d^3\mathbf{r}_4^f d^3\boldsymbol{\xi}_{21}^i d^3\boldsymbol{\xi}_{43}^i d^3\mathbf{R}_{d1}^i d^3\mathbf{R}_{d2}^i d^{3N-3}\{\mathbf{R}\} \quad (41)$$

where we have defined the relative coordinates

$$\boldsymbol{\xi}_{21}^i = \mathbf{r}_2^i - \mathbf{r}_1^i \quad \boldsymbol{\xi}_{43}^i = \mathbf{r}_4^i - \mathbf{r}_3^i \quad \boldsymbol{\xi}_{32}^f = \mathbf{r}_3^f - \mathbf{r}_2^f \quad \boldsymbol{\xi}_{21}^f = \mathbf{r}_2^f - \mathbf{r}_1^f \quad (42)$$

and the center of mass coordinates

$$\mathbf{R}_{d1}^i = \frac{\mathbf{r}_1^i + \mathbf{r}_2^i}{2} \quad \mathbf{R}_{d2}^i = \frac{\mathbf{r}_3^i + \mathbf{r}_4^i}{2} \quad \mathbf{R}_{3He}^f = \frac{\mathbf{r}_1^f + \mathbf{r}_2^f + \mathbf{r}_3^f}{3} \quad (43)$$

### B. Deuteron-deuteron separation

When the two deuterons are close enough for strong force interactions to take place, then the Coulomb repulsion is sufficiently strong that this interaction dominates over the forces from other atoms. Although we can use a phonon description in this case, it would not be the most natural, and the Coulomb forces would require the presence of very high-order phonon operators. Hence, it may be more convenient to adopt the point of view that the

two deuterons appear to the lattice as an equivalent  ${}^4\text{He}$  nucleus when they are a few fermis apart. The separation between them may best be handled then as part of the microscopic nuclear problem. In this case, we may write

$$\begin{aligned}
I = & \int \left[ \phi_{3He}(\xi_{32}^f, \xi_{21}^f) F_{3,1}^L \left( \mathbf{R}_{3He}^f, \mathbf{r}_4^f, \{\mathbf{R}\} \right) \right]^* V(\xi_{21}^f) \phi_d(\xi_{21}^i) \phi_d(\xi_{43}^i) \\
& F_{2,2}^L \left( \mathbf{R}_{4He}^i - \frac{1}{2} \mathbf{r}_{dd}^i, \mathbf{R}_{4He}^i + \frac{1}{2} \mathbf{r}_{dd}^i, \{\mathbf{R}\} \right) \delta^{(3)} \left( -\frac{1}{3} \xi_{32}^f - \frac{2}{3} \xi_{21}^f + \mathbf{R}_{3He}^f - \left( -\frac{1}{2} \xi_{21}^i + \mathbf{R}_{4He}^i - \frac{1}{2} \mathbf{r}_{dd}^i \right) \right) \\
& \delta^{(3)} \left( -\frac{1}{3} \xi_{32}^f + \frac{1}{3} \xi_{21}^f + \mathbf{R}_{3He}^f - \left( \frac{1}{2} \xi_{21}^i + \mathbf{R}_{4He}^i - \frac{1}{2} \mathbf{r}_{dd}^i \right) \right) \\
& \delta^{(3)} \left( \frac{2}{3} \xi_{32}^f + \frac{1}{3} \xi_{21}^f + \mathbf{R}_{3He}^f - \left( -\frac{1}{2} \xi_{43}^i + \mathbf{R}_{4He}^i + \frac{1}{2} \mathbf{r}_{dd}^i \right) \right) \\
& \delta^{(3)} \left( \mathbf{r}_4^f - \left( \frac{1}{2} \xi_{43}^i + \mathbf{R}_{4He}^i + \frac{1}{2} \mathbf{r}_{dd}^i \right) \right) d^3 \xi_{32}^f d^3 \xi_{21}^f d^3 \mathbf{R}_{3He}^f d^3 \mathbf{r}_4^f d^3 \xi_{21}^i d^3 \xi_{43}^i d^3 \mathbf{R}_{4He}^i d^3 \mathbf{r}_{dd}^i d^{3N-3} \{\mathbf{R}\}
\end{aligned} \tag{44}$$

In writing this, we have made use of the initial state relative and center of mass coordinates

$$\mathbf{R}_{4He}^i = \frac{1}{2} (\mathbf{R}_{d1}^i + \mathbf{R}_{d2}^i) \quad \mathbf{r}_{dd}^i = \mathbf{R}_{d2}^i - \mathbf{R}_{d1}^i \tag{45}$$

Note that in casting the matrix element in this way we are not assuming that the microscopic  ${}^4\text{He}$  nuclear wavefunction is the same as the microscopic nuclear wavefunction for two deuterons. Instead, we recognize in these expressions that there is little difference from the point of view of the rest of the lattice between two deuterons localized on the fermi scale (which the rest of the lattice sees as a charge 2 and mass 4 object), and a  ${}^4\text{He}$  nucleus (which the rest of the lattice also sees as a charge 2 and mass 4 object). Due to the Coulomb repulsion between the two deuterons when they are close, the associated relative wavefunction is far into a tunneling regime. We have the choice to describe this tunneling in terms of deuteron coordinates as phonon operators, which is complicated, or else to describe this tunneling via a relative nuclear coordinate based on a  ${}^4\text{He}$  center of mass coordinate, which is much simpler. The formal problem is not changed with this replacement, although the approximations used in the evaluation of the resulting expressions could be different.

### C. Transformation to phonon coordinates

We are now in a position to make the transformation to phonon coordinates. In the initial state, a nuclear center of mass coordinates can be expressed in terms of phonon coordinates in general according to

$$\hat{\mathbf{R}}_j^i = \mathbf{R}_j^{i,0} + \sum_m \mathbf{u}_j^i[m] \hat{q}_m^i \tag{46}$$

Consequently, we may transform from initial state center of mass coordinates to initial state phonon coordinates

$$\mathbf{R}_{4He}^i, \{\mathbf{R}\} \rightarrow \mathbf{R}_L^i, \{q^i\} \quad (47)$$

where  $\mathbf{R}_L^i$  is the center of mass of the initial state lattice. A similar transformation is possible for the final state center of mass coordinates, which we indicate by

$$\mathbf{R}_{3He}^f, \{\mathbf{R}\} \rightarrow \mathbf{R}_L^f, \{q^f\} \quad (48)$$

where  $\mathbf{R}_L^f$  is the center of mass of the final state lattice.

$$\begin{aligned} I = & \int \left[ \phi_{3He}(\boldsymbol{\xi}_{32}^f, \boldsymbol{\xi}_{21}^f) F_{3,1}^L \left( \hat{\mathbf{R}}_{3He}^f, \mathbf{r}_4^f, \{\hat{\mathbf{R}}^f\} \right) \right]^* V(\boldsymbol{\xi}_{21}^f) \phi_d(\boldsymbol{\xi}_{21}^i) \phi_d(\boldsymbol{\xi}_{43}^i) \\ & F_{2,2}^L \left( \hat{\mathbf{R}}_{4He}^i - \frac{1}{2} \mathbf{r}_{dd}^i, \hat{\mathbf{R}}_{4He}^i + \frac{1}{2} \mathbf{r}_{dd}^i, \{\hat{\mathbf{R}}^i\} \right) \delta^{(3)} \left( \mathbf{R}_L^f - \mathbf{R}_L^i \right) \\ & \delta^{(3)} \left( -\frac{1}{3} \boldsymbol{\xi}_{32}^f - \frac{2}{3} \boldsymbol{\xi}_{21}^f + \hat{\mathbf{R}}_{3He}^f - \left( -\frac{1}{2} \boldsymbol{\xi}_{21}^i + \hat{\mathbf{R}}_{4He}^i - \frac{1}{2} \mathbf{r}_{dd}^i \right) \right) \\ & \delta^{(3)} \left( -\frac{1}{3} \boldsymbol{\xi}_{32}^f + \frac{1}{3} \boldsymbol{\xi}_{21}^f + \hat{\mathbf{R}}_{3He}^f - \left( \frac{1}{2} \boldsymbol{\xi}_{21}^i + \hat{\mathbf{R}}_{4He}^i - \frac{1}{2} \mathbf{r}_{dd}^i \right) \right) \\ & \delta^{(3)} \left( \frac{2}{3} \boldsymbol{\xi}_{32}^f + \frac{1}{3} \boldsymbol{\xi}_{21}^f + \hat{\mathbf{R}}_{3He}^f - \left( -\frac{1}{2} \boldsymbol{\xi}_{43}^i + \hat{\mathbf{R}}_{4He}^i + \frac{1}{2} \mathbf{r}_{dd}^i \right) \right) \\ & \delta^{(3)} \left( \mathbf{r}_4^f - \left( \frac{1}{2} \boldsymbol{\xi}_{43}^i + \hat{\mathbf{R}}_{4He}^i + \frac{1}{2} \mathbf{r}_{dd}^i \right) \right) \delta^{(3N-3)}(\mathbf{q}^f - \bar{\mathbf{A}} \cdot \mathbf{q}^i - \mathbf{b}) \\ & d^3 \mathbf{R}_L^f d^3 \mathbf{R}_L^i d^3 \boldsymbol{\xi}_{32}^f d^3 \boldsymbol{\xi}_{21}^f d^3 \mathbf{r}_4^f d^3 \boldsymbol{\xi}_{21}^i d^3 \boldsymbol{\xi}_{43}^i d^3 \mathbf{r}_{dd}^i d^{3N-3} \mathbf{q}^f d^{3N-3} \mathbf{q}^i \end{aligned} \quad (49)$$

where

$$\hat{\mathbf{R}}_{3He}^f = \hat{\mathbf{R}}_{3He}^f(\mathbf{q}^f, \mathbf{R}_L^f) \quad (50)$$

$$\hat{\mathbf{R}}_k^f = \hat{\mathbf{R}}_k^f(\mathbf{q}^f, \mathbf{R}_L^f) \quad (51)$$

$$\hat{\mathbf{R}}_{4He}^i = \hat{\mathbf{R}}_{4He}^i(\mathbf{q}^i, \mathbf{R}_L^i) \quad (52)$$

$$\hat{\mathbf{R}}_k^i = \hat{\mathbf{R}}_k^i(\mathbf{q}^i, \mathbf{R}_L^i) \quad (53)$$

#### D. Integral in terms of generalized lattice wavefunctions

The generalized lattice channel separation factors are the same as lattice wavefunctions augmented with additional degrees of freedom. Let us adopt a notation of the form

$$F_{2,2}^L \left( \hat{\mathbf{R}}_{4He}^i - \frac{1}{2} \mathbf{r}_{dd}^i, \hat{\mathbf{R}}_{4He}^i + \frac{1}{2} \mathbf{r}_{dd}^i, \{\hat{\mathbf{R}}^i\} \right) \rightarrow \Psi_i^L(\mathbf{q}^i, \mathbf{r}_{dd}^i) \quad (54)$$

$$F_{3,1}^L \left( \hat{\mathbf{R}}_{3He}^f, \mathbf{r}_4^f, \{\hat{\mathbf{R}}^f\} \right) \rightarrow \Psi_f^L(\mathbf{q}^f, \mathbf{r}_4^f) \quad (55)$$

The generalized lattice wavefunctions include an explicit dependence on phonon coordinates, as well as an explicit dependence on a microscopic nuclear degree of freedom. In the initial state, this extra degree of freedom is the deuteron-deuteron separation; in the final state it is the position of the neutron. Implicit in this description is an assumption that the lattice center of mass is preserved, which is an additional assumption here that is consistent with our focus on phonon exchange (we do not mean to imply here that no coupling is possible with the lattice center of mass coordinate). With this notation, we may write

$$I = \int \left[ \Psi_f^L(\mathbf{q}^f, \mathbf{r}_4^f) \right]^* \hat{v}_{fi}(\mathbf{q}^f, \mathbf{q}^i) \Psi_i^L(\mathbf{q}^i, \mathbf{r}_{dd}^i) \delta^{(3N-3)}(\mathbf{q}^f - \mathbf{A} \cdot \mathbf{q}^i - \mathbf{b}) d^3 \mathbf{r}_4^f d^3 \mathbf{r}_{dd}^i d\mathbf{q}^f d\mathbf{q}^i \quad (56)$$

where the interaction potential is

$$\begin{aligned} \hat{v}_{fi}(\mathbf{q}^f, \mathbf{q}^i) = & \int \left[ \phi_{3He}^f(\boldsymbol{\xi}_{32}^f, \boldsymbol{\xi}_{21}^f) \right]^* V(\boldsymbol{\xi}_{21}^f) \phi_d(\boldsymbol{\xi}_{21}^i) \phi_d(\boldsymbol{\xi}_{43}^i) \\ & \delta^{(3)} \left( -\frac{1}{3} \boldsymbol{\xi}_{32}^f - \frac{2}{3} \boldsymbol{\xi}_{21}^f + \hat{\mathbf{R}}_{3He}^f - \left( -\frac{1}{2} \boldsymbol{\xi}_{21}^i + \hat{\mathbf{R}}_{4He}^i - \frac{1}{2} \mathbf{r}_{dd}^i \right) \right) \\ & \delta^{(3)} \left( -\frac{1}{3} \boldsymbol{\xi}_{32}^f + \frac{1}{3} \boldsymbol{\xi}_{21}^f + \hat{\mathbf{R}}_{3He}^f - \left( \frac{1}{2} \boldsymbol{\xi}_{21}^i + \hat{\mathbf{R}}_{4He}^i - \frac{1}{2} \mathbf{r}_{dd}^i \right) \right) \\ & \delta^{(3)} \left( \frac{2}{3} \boldsymbol{\xi}_{32}^f + \frac{1}{3} \boldsymbol{\xi}_{21}^f + \hat{\mathbf{R}}_{3He}^f - \left( -\frac{1}{2} \boldsymbol{\xi}_{43}^i + \hat{\mathbf{R}}_{4He}^i + \frac{1}{2} \mathbf{r}_{dd}^i \right) \right) \\ & \delta^{(3)} \left( \mathbf{r}_4^f - \left( \frac{1}{2} \boldsymbol{\xi}_{43}^i + \hat{\mathbf{R}}_{4He}^i + \frac{1}{2} \mathbf{r}_{dd}^i \right) \right) d^3 \boldsymbol{\xi}_{32}^f d^3 \boldsymbol{\xi}_{21}^f d^3 \boldsymbol{\xi}_{21}^i d^3 \boldsymbol{\xi}_{43}^i \end{aligned} \quad (57)$$

We may integrate over the final state phonon coordinates to obtain

$$I = \int \left[ \Psi_f^L(\mathbf{q}^f, \mathbf{r}_4^f) \right]^* \hat{v}_{fi}(\mathbf{q}^f, \mathbf{q}^i) \Psi_i^L(\mathbf{q}^i, \mathbf{r}_{dd}^i) d^3 \mathbf{r}_4^f d^3 \mathbf{r}_{dd}^i d\mathbf{q}^i \quad (58)$$

in which the final state phonon coordinates are expressed in terms of initial state coordinates as

$$\mathbf{q}^f = \mathbf{A} \cdot \mathbf{q}^i + \mathbf{b} \quad (59)$$

Equations (57) and (58) are the primary results that we find in the particular integral involved in the specific deuteron-deuteron matrix element considered as our example. Similar results can be readily obtained for other integrals appearing in this matrix element, and also for other matrix elements as well.

## VII. CONCLUSIONS

The analysis presented in this paper is motivated by claims of excess power production in experiments involving metal deuterides that have been reported over the years since the original claim of Fleischmann and Pons in 1989. The existence of such an effect implies new physical mechanisms, in particular mechanisms which lead to a coupling between condensed matter degrees of freedom and nuclear degrees of freedom. There has been confusion and conjecture about how energy or angular momentum exchange with the lattice works, and no relevant formulation or calculations have been reported in the mainstream literature. In recent years, our focus has been on a particular scheme involving excitation transfer, idealized models for which are discussed in detail in a recent manuscript.<sup>9</sup> The formulation discussed in this paper leads to formulas that can be used for a quantitative evaluation of this model, and other models that have been proposed which also involve coupling with phonons.

The nuclear part of the calculation requires spin and isospin degrees of freedom in addition to the spatial degrees of freedom. We developed nuclear wavefunctions based on Yamanouchi basis functions for each degree of freedom individually, which allows us to integrate out the spin and isospin degrees of freedom separately in a convenient way. This leads to a straightforward expansion of the interaction matrix element in terms of a sum of spatial integrals which contain different permutations of particle numbering.

The lattice part of the problem comes into the calculation initially as spectator degrees of freedom in the generalized channel separation factor. In essence, the microscopic part of the calculation at this level is completely equivalent to the vacuum calculation, since the spectator nuclei are not involved locally in the strong force interaction. The lattice does come into the problem in a more fundamental way when we replace the nuclear center of mass degrees of freedom with phonon coordinates. Since the reacting nuclei in this formulation are taken to be part of the lattice in both initial and final states, the lattice is changed as a result of the reaction. We chose a description in which both the initial and final state product nuclei are assumed to be included in the associated lattice definitions. This leads to integrals which contain both initial state and final state lattice wavefunctions, where the lattice structure is different in the two cases.

## APPENDIX A: THE NUCLEAR POTENTIAL

We make use of the Hamada-Johnston potential as our model nuclear potential in this paper. It is one of the simplest isospin-preserving nuclear potentials to give reasonable results. The Hamada-Johnston potential between nucleon 1 and nucleon 2 can be written as

$$V_{HJ}(1, 2) = V_C(1, 2) + V_T(1, 2)S_{12} + V_{LS}(1, 2)(\mathbf{L} \cdot \mathbf{S}) + V_{LL}(1, 2)L_{12} \quad (\text{A1})$$

where  $\mathbf{L}$  and  $\mathbf{S}$  are the relative angular momentum and the total spin of the two nuclei. The individual potentials are defined as

$$\begin{aligned} V_C(1, 2) &= (\boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2) (\boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2) y_C(\mu r_{12}) \\ V_T(1, 2) &= (\boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2) y_T(\mu r_{12}) \\ S_{12} &= 3 \frac{(\boldsymbol{\sigma}_1 \cdot \mathbf{r}_{12})(\boldsymbol{\sigma}_2 \cdot \mathbf{r}_{12})}{r_{12}^2} - \boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2 \\ V_{LS}(1, 2) &= y_{LS}(\mu r_{12})(\mathbf{L} \cdot \mathbf{S}) \\ V_{LL}(1, 2) &= y_{LL}(\mu r_{12}) \\ L_{12} &= (\boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2)\mathbf{L}^2 - \frac{1}{2}(\boldsymbol{\sigma}_1 \cdot \mathbf{L})(\boldsymbol{\sigma}_2 \cdot \mathbf{L}) - \frac{1}{2}(\boldsymbol{\sigma}_2 \cdot \mathbf{L})(\boldsymbol{\sigma}_1 \cdot \mathbf{L}) \end{aligned}$$

The spatial functions are given by

$$\begin{aligned} y_C^\alpha(x) &= 0.08 \frac{m_\pi c^2}{3} Y(x) \{1 + a_C^\alpha Y(x) + b_C^\alpha Y^2(x)\} \\ y_T^\alpha(x) &= 0.08 \frac{m_\pi c^2}{3} Z(x) \{1 + a_T^\alpha Y(x) + b_T^\alpha Y^2(x)\} \\ y_{LS}^\alpha(x) &= m_\pi c^2 G_{LS}^\alpha Y^2(x) \{1 + b_{LS}^\alpha Y(x)\} \\ y_{LL}^\alpha(x) &= m_\pi c^2 G_{LL}^\alpha x^{-2} Z(x) \{1 + a_{LL}^\alpha Y(x) + b_{LL}^\alpha Y^2(x)\} \end{aligned}$$

where  $m_\pi$  is the pion mass,  $\alpha$  stands for odd-singlet(*os*), even-singlet(*es*), odd-triplet(*ot*) or even-triplet(*et*). The functions  $Y(x)$  and  $Z(x)$  have the definitions

$$Y(x) = \frac{e^{-x}}{x} \quad Z(x) = \left(1 + \frac{3}{x} + \frac{3}{x^2}\right) Y(x)$$

## APPENDIX B: SYMMETRIC GROUP

The symmetric group  $S(n)$ , the group of permutations of  $n$  objects, plays an important role in our calculation. It does so, in three important ways

- Clebsch-Gordan coefficients are used to construct the antisymmetric wavefunctions.
- Schur-Weyl duality lets us build wavefunctions with a well-defined spin (and isospin) and which also transform as Yamanouchi basis vectors under  $S(4)$ .
- Induction coefficients of  $S(4)$  are utilized to construct Yamanouchi basis vectors for the spatial part.

In quantum mechanics, we are familiar with the transformation properties of the spherical harmonics. In the case of  $Y_{lm}$ 's the  $l$  labels the irreducible representation of  $SO(3)$  and  $m$  labels the basis vector. Similarly for the symmetric group, we get two labels: the Young diagrams and the Yamanouchi symbols<sup>20,21</sup>, where the Young diagrams label the irreducible representation of  $S(4)$  and the Yamanouchi symbols label the basis vectors. The index scheme we use for the Yamanouchi symbols is defined in Table I.

TABLE I: Definition of indices for the Yamanouchi symbols

Yamanouchi Symbol	index	Yamanouchi symbol	index
4321	1	2121	6
3211	2	2111	7
3121	3	1211	8
1321	4	1121	9
2211	5	1111	10

### 1. Clebsch-Gordan coefficients

The general formula for constructing antisymmetric wavefunctions is given by

$$\Psi([f], [f'], [f'']) = \sum_{Y, \tilde{Y}} C_{[\tilde{f}], \tilde{Y}; [f], Y}^{[1^4], 1} R([\tilde{f}], \tilde{Y}) \sum_{Y', Y''} C_{[f']Y'; [f'']Y''}^{[f], Y} S([f'], Y') T([f''], Y'') \quad (\text{B1})$$

where the  $C$ 's are the Clebsch-Gordan coefficients of  $S(4)$ ,  $[f]$ 's are the Young diagrams,  $Y$ 's are the Yamanouchi symbols,  $\tilde{f}$  and  $\tilde{Y}$  are the conjugate Young diagrams and Yamanouchi symbols and  $[1^4]$  represents the completely antisymmetric one dimensional representation with one Yamanouchi basis vector (index 1). The Clebsch-Gordan coefficients of  $S(4)$  are available in the literature<sup>20,21,22,23</sup>.



As a specific example, we construct the basis function  $\Psi_i = \Psi_6$ . Using our indexing scheme of Table I above and Table 4.13 of Chen et al<sup>23</sup>, we see that

$$C_{10,5}^5 = 1 \quad C_{10,6}^6 = 1 \quad (\text{B2})$$

Hence the spin-isospin part of Equation B1 yields

$$(st)_5 = s_{10}t_5 \quad (st)_6 = s_{10}t_6 \quad (\text{B3})$$

where the subscripts in  $(st)_5$  or  $(st)_6$  again refer to the Yamanouchi basis for the particular spin-isospin combination. In addition, we have

$$C_{5,6}^1 = \frac{1}{\sqrt{2}} \quad C_{6,5}^1 = -\frac{1}{\sqrt{2}} \quad (\text{B4})$$

Therefore, the totally antisymmetric wavefunction can be written as

$$\Psi_6 = \frac{1}{\sqrt{2}}\psi_5(st)_6 - \frac{1}{\sqrt{2}}\psi_6(st)_5 = \frac{1}{\sqrt{2}}[\psi_5 s_{10}t_6 - \psi_6 s_{10}t_5] \quad (\text{B5})$$

## 2. Schur-Weyl duality

The Schur-Weyl duality relates certain representations of  $SU(m)$  or  $GL(m)$  to the representations of  $S(n)$ . For our purposes, since we are only interested in the spin-half (or isospin-half) case, the Schur-Weyl duality is particularly simple. It states that there are no spin (or isospin) wavefunctions corresponding to the index 1,2,3 or 4. It also allows us to construct the rest of the wavefunctions very simply. In the usual spectroscopic notation, with the nucleon number as a subscript and  $\sigma$  referring to spin angular momentum.

$$\begin{aligned} s_5 &= |\sigma_1\sigma_2(S_{12}=1), \sigma_3(S_{123}=\frac{1}{2}), \sigma_4 S=0\rangle \\ s_6 &= |\sigma_1\sigma_2(S_{12}=0), \sigma_3(S_{123}=\frac{1}{2}), \sigma_4 S=0\rangle \\ s_7 &= |\sigma_1\sigma_2(S_{12}=1), \sigma_3(S_{123}=\frac{3}{2}), \sigma_4 S=1\rangle \\ s_8 &= |\sigma_1\sigma_2(S_{12}=1), \sigma_3(S_{123}=\frac{1}{2}), \sigma_4 S=1\rangle \\ s_9 &= |\sigma_1\sigma_2(S_{12}=0), \sigma_3(S_{123}=\frac{1}{2}), \sigma_4 S=1\rangle \\ s_{10} &= |\sigma_1\sigma_2(S_{12}=1), \sigma_3(S_{123}=\frac{3}{2}), \sigma_4 S=2\rangle \end{aligned} \quad (\text{B6})$$

Here on the RHS, we are suppressing the value of  $M_S$  because different  $M_S$  values transform in the same way under the symmetric group. Exactly the same results apply to the isospin wavefunctions, since they are also angular momentum 1/2 representations of  $SU(2)$ .

### 3. Induction Coefficients

In the previous subsection we explicitly constructed the spin/isospin Yamanouchi wavefunctions using angular momentum addition. We still have to construct the spatial Yamanouchi wavefunctions. One way to do it is to use induction coefficients of the symmetric group, which are tabulated and discussed in Chen et al.<sup>23</sup>. The relevant formula for our purposes is

$$\psi^n([f], Y^f) = \sum_{Y^g, Y^h, \omega} S_{[g], Y^g; [h], Y^h; \omega}^{[f], Y^f} \psi^{n1}([g], Y^g, \omega_1) \psi^{n2}([h], Y^h, \omega_2) \quad (\text{B7})$$

Here  $n = n1 + n2$ ,  $[f]$  and  $Y^f$  are the Young diagram and the Yamanouchi symbol for an  $n$ -particle spatial wavefunction,  $[g]$  and  $Y^g$  are the Young diagram and Yamanouchi symbol for the  $n1$ -particle wavefunction and  $[h]$  and  $Y^h$  are the Young diagram and Yamanouchi symbol for the  $n2$ -particle wavefunction and  $\omega = (\omega_1, \omega_2)$  represents a permutation of  $\{1, 2, \dots, n\}$ .

As a concrete example let us consider  $n = 4$  case with  $n1 = n2 = 2$ . Suppose we want to construct a  $\psi_6$ , starting with two two-body spatial wavefunctions,  $\phi$  and  $\phi'$ , which are completely symmetric. Hence the summation over the Yamanouchi symbols is trivial and we only need to sum over various  $\omega$ 's corresponding to different orderings of  $\{1, 2, 3, 4\}$ . We can use Table 4.17 of Chen et al.<sup>23</sup> to see that (suppressing the trivial Yamanouchi symbols)

$$S_{\{2,3,1,4\}}^6 = -\frac{1}{2} \quad S_{\{1,4,2,3\}}^6 = -\frac{1}{2} \quad S_{\{1,3,2,4\}}^6 = \frac{1}{2} \quad S_{\{2,4,1,3\}}^6 = \frac{1}{2} \quad (\text{B8})$$

Hence

$$\psi_6 = \frac{1}{2} [-\phi(2, 3)\phi'(1, 4) - \phi(1, 4)\phi'(2, 3) + \phi(1, 3)\phi'(2, 4) + \phi(2, 4)\phi'(1, 3)] \quad (\text{B9})$$

We can use this approach to develop a complete set of results needed for the case of two deuterons as used in this paper. For the initial state, we may write

$$\begin{aligned} \psi_5 &= \frac{1}{\sqrt{12}} [2\psi(12; 34) + 2\psi(34; 21) - \psi(23; 14) - \psi(14; 23) - \psi(13; 24) - \psi(24; 13)] \\ \psi_6 &= \frac{1}{2} [-\psi(23; 14) - \psi(14; 23) + \psi(13; 24) + \psi(24; 13)] \end{aligned} \quad (\text{B10})$$

where  $\psi(12; 34)$  is any spatial wavefunction which is symmetric under the  $1 \leftrightarrow 2$  and  $3 \leftrightarrow 4$  exchange. For the final state, we are using a three-nucleon body and a one nucleon body. The Yamanouchi wavefunctions are

$$\begin{aligned}
\psi_{10} &= \frac{1}{2} [\psi(123; 4) + \psi(124; 3) + \psi(134; 2) + \psi(234; 1)] \\
\psi_7 &= \frac{1}{\sqrt{12}} [3\psi(123; 4) - \psi(124; 3) - \psi(134; 2) - \psi(234; 1)] \\
\psi_8 &= \frac{1}{\sqrt{6}} [2\psi(124; 3) - \psi(134; 2) - \psi(234; 1)] \\
\psi_9 &= \frac{1}{\sqrt{2}} [\psi(134; 2) - \psi(234; 1)]
\end{aligned} \tag{B11}$$

where the  $\psi(123; 4)$  is any wavefunction symmetric under any permutation of  $\{1, 2, 3\}$ .

Hence we see that by using induction coefficients, we can take spatial wavefunctions which belongs to certain representations of subgroups of  $S(4)$  and use them to construct Yamanouchi basis vectors e.g. for the case of two deuterons, we started with  $\psi(12; 34)$  which is symmetric under the exchange of  $1 \leftrightarrow 2$  or  $3 \leftrightarrow 4$ , and constructed spatial wavefunctions with Yamanouchi basis index 5 or 6.

## APPENDIX C: YAMANOUCI BASIS STATES

Below we explicitly write down the  $T = 0$  basis states. Please note that the subscripts on the LHS of the equations are merely ways of enumerating the possible wavefunctions, where as the subscripts on the RHS are the indices for the Yamanouchi symbols (see Table I).

**S = 0**

$$\begin{aligned}\Psi_1 &= \psi_{10} \frac{1}{\sqrt{2}} [s_5 t_6 - s_6 t_5] \\ \Psi_2 &= \psi_1 \frac{1}{\sqrt{2}} [s_5 t_5 + s_6 t_6] \\ \Psi_3 &= -\frac{1}{2} \psi_5 [s_5 t_6 + s_6 t_5] - \frac{1}{2} \psi_6 [s_5 t_5 - s_6 t_6]\end{aligned}$$

**S = 1**

$$\begin{aligned}\Psi_4 &= \frac{1}{\sqrt{6}} \psi_7 [s_8 t_6 - s_9 t_5] + \frac{1}{2\sqrt{3}} \psi_8 [\sqrt{2} s_7 t_6 + s_8 t_6 + s_9 t_5] + \\ &\quad \frac{1}{2\sqrt{3}} \psi_9 [-\sqrt{2} s_7 t_5 + s_8 t_5 - s_9 t_6] \\ \Psi_5 &= \frac{1}{2\sqrt{3}} \psi_2 [\sqrt{2} s_7 t_6 - s_8 t_6 - s_9 t_5] - \\ &\quad \frac{1}{2\sqrt{3}} \psi_3 [\sqrt{2} s_7 t_5 + s_8 t_5 - s_9 t_6] + \frac{1}{\sqrt{6}} \psi_4 [s_8 t_5 + s_9 t_6]\end{aligned}$$

**S = 2**

$$\Psi_6 = \frac{1}{\sqrt{2}} [\psi_5 s_{10} t_6 - \psi_6 s_{10} t_5]$$

## APPENDIX D: THE TENSOR MATRIX ELEMENT

We have calculated a complete set of such Yamanouchi matrix elements for the  $T = 0$  case. There are too many cases to be presented here. We therefore focus on a specific example by calculating the tensor force matrix element of  $\Psi_1(M_s = 0)$  and  $\Psi_6(M_s = 1)$ . The main issue with all these calculations is that the parameters in most of the nuclear potentials are fit separately to spin singlet-triplet and even-odd spatial parity (for example, in the Hamada-Johnston potential the  $y$  functions are parameterized by  $a$  and  $b$  parameters, which depend on the spin and parity). The most convenient way of dealing with these issues is to use projection operators to separate the various parity and spin channels. However we can, without the use of projection operators, directly exploit the properties of the interaction and the wavefunctions to evaluate these matrix elements.

### 1. Exchange properties of the interaction and wavefunctions

First of all, since we are using completely antisymmetric wavefunctions, the tensor part of the matrix element calculation simplifies to

$$\begin{aligned} \left\langle \Psi_f \left| \sum_{\alpha < \beta} V_T(\alpha, \beta) S_{\alpha\beta} \right| \Psi_i \right\rangle &= \langle \Psi_1(0) | \sum_{1 \leq i < j \leq 4} V_T(i, j) S_{ij} | \Psi_6(1) \rangle \\ &= 6 \langle \Psi_1(0) | V_T(1, 2) S_{12} | \Psi_6(1) \rangle \end{aligned} \quad (\text{D1})$$

Here the values 0 and 1 in the parentheses represent the  $M_S$  values of the initial and final wavefunctions. So now, as discussed in the main text, the tensor interaction can be evaluated by

$$\begin{aligned} \left\langle \Psi_f \left| \sum_{\alpha < \beta} V_T(\alpha, \beta) S_{\alpha\beta} \right| \Psi_i \right\rangle &= 3 \left[ \langle s_5 t_6 \psi_{10} | V_T(1, 2) S_{12} | s_{10} t_6 \psi_5 \rangle - \langle s_5 t_6 \psi_{10} | V_T(1, 2) S_{12} | s_{10} t_5 \psi_6 \rangle \right. \\ &\quad \left. - \langle s_6 t_5 \psi_{10} | V_T(1, 2) S_{12} | s_{10} t_6 \psi_5 \rangle + \langle s_6 t_5 \psi_{10} | V_T(1, 2) S_{12} | s_{10} t_5 \psi_6 \rangle \right] \end{aligned} \quad (\text{D2})$$

From the explicit form of  $V_T(1, 2) S_{12}$ , we can see that it is symmetric under the exchange  $1 \leftrightarrow 2$ , individually for spin, isospin and space parts. If we look at the explicit form of the spin wavefunctions in Appendix B we can see that since particles 1 and 2 couple to form a triplet,  $s_5, s_7, s_8$  and  $s_{10}$  are even under  $1 \leftrightarrow 2$ . Similarly since particles 1 and 2 couple to form a singlet,  $s_6$  and  $s_9$  are odd under  $1 \leftrightarrow 2$ . The same applies to the isospin wavefunctions. Being even or odd under the exchange  $1 \leftrightarrow 2$  in this case has nothing to do with angular momentum algebra, but is a property of the Yamanouchi symbol. Hence the spatial wavefunctions  $\psi_5, \psi_7, \psi_8$  and  $\psi_{10}$  are even under  $1 \leftrightarrow 2$  and  $\psi_6$  and  $\psi_9$  are odd under

$1 \leftrightarrow 2$ . As a concrete example, this can easily be seen by explicitly looking at the  $\psi_6$  from Appendix B

$$\psi_6 = \frac{1}{2} [-\phi(2, 3)\phi'(1, 4) - \phi(1, 4)\phi'(2, 3) + \phi(1, 3)\phi'(2, 4) + \phi(2, 4)\phi'(1, 3)] \quad (\text{D3})$$

This  $\psi_6$ , under the exchange  $1 \leftrightarrow 2$ , transforms to

$$\psi_6 \rightarrow \frac{1}{2} [-\phi(1, 3)\phi'(2, 4) - \phi(2, 4)\phi'(1, 3) + \phi(2, 3)\phi'(1, 4) + \phi(1, 4)\phi'(2, 3)] = -\psi_6 \quad (\text{D4})$$

Because of the symmetry of the interaction under  $1 \leftrightarrow 2$ , individually for space, spin and isospin parts, we only get non-zero couplings when the space, spin and isospin have the same parity (under  $1 \leftrightarrow 2$ ) for both the initial and the final wavefunction. Hence we can see that

$$\langle s_5 t_6 \psi_{10} | V_T(1, 2) S_{12} | s_{10} t_5 \psi_6 \rangle = 0$$

$$\langle s_6 t_5 \psi_{10} | V_T(1, 2) S_{12} | s_{10} t_6 \psi_5 \rangle = 0$$

$$\langle s_6 t_5 \psi_{10} | V_T(1, 2) S_{12} | s_{10} t_5 \psi_6 \rangle = 0$$

The only non-zero matrix element is  $\langle s_5 t_6 \psi_{10} | V_T(1, 2) S_{12} | s_{10} t_6 \psi_5 \rangle$ .

## 2. Matrix element calculation

We have reduced our matrix element calculation to just calculating  $\langle s_5 t_6 \psi_{10} | V_T(1, 2) S_{12} | s_{10} t_6 \psi_5 \rangle$ . We can evaluate the spin and isospin pieces separately

$$\langle t_6 | \tau_1 \cdot \tau_2 | t_6 \rangle = -3 \quad (\text{D5})$$

$$\langle s_5(M_S = 0) | S_{12} | s_{10}(M_S = 1) \rangle = -2\sqrt{3} z_{12} \frac{x_{12} + iy_{12}}{r_{12}^2} \quad (\text{D6})$$

Since the  $s_{10}$  and  $s_5$  are triplets and  $\psi_{10}$  and  $\psi_5$  are even, the  $y_T(\mu r_{12})$  should be the one parameterized by even parity and triplet spin. Hence  $y_T(\mu r_{12}) = y_T^{et}(\mu r_{12})$  where *et* stands for “even, triplet”.

We can assemble these results to obtain

$$\left\langle \Psi_1(0) \left| \sum_{1 \leq i < j \leq 4} V_T(i, j) S_{i,j} \right| \Psi_6(1) \right\rangle = 18\sqrt{3} \int \psi_{10}^* \left[ \frac{(x_{12} + iy_{12}) z_{12} y_T^{et}(\mu r_{12})}{r_{12}^2} \right] \psi_5 d^3 \mathbf{r}_1 \cdots d^3 \mathbf{r}_4 \quad (\text{D7})$$

where  $\psi_{10}^* = \psi_{10}^*(\mathbf{r}_1, \dots, \mathbf{r}_4)$  and  $\psi_5 = \psi_5(\mathbf{r}_1, \dots, \mathbf{r}_4)$  are functions of spatial coordinates alone.

## APPENDIX E: VACUUM CASE ANTISYMMETRIZATION

In Appendix D we saw that it was straightforward to calculate the matrix element of the tensor force in terms of the Yamanouchi basis. This is in general true for all nuclear interactions. Perhaps the simplest way of carrying out realistic physical calculations is to express initial and final state wavefunctions in terms of the Yamanouchi basis. Then we can use the Yamanouchi basis matrix element results to calculate the nuclear matrix elements with physical initial and final states.

For an isospin preserving,  $T = 0$  reaction, in which two deuterons interact to form a three-nucleon body and a one nucleon body the relevant states are:

- $\Psi_{2,2}$ : One initial  $2 + 2$  state of two deuterons in a quintet spin 2 state. We should in general consider the deuterons to be in a singlet or triplet as well. However, we are focusing on a single example here. In this enumeration of states, we suppress the various  $M_S$  values.
- $\Psi_{3,1}$ : Two final  $3 + 1$  states (since these can be singlets or triplets). These are a linear superpositions of the  ${}^3H + p$  and  ${}^3He + n$  states.

### 1. Physical wavefunctions

The wavefunctions discussed above are formal Yamanouchi objects which are very general. We need to focus on specific wavefunctions for the different mass 4 ( $T = 0$ ) channels in order to proceed. For simplicity, we adopt a wavefunction for two deuterons that are in a quintet (spin 2) state. In this case, we can use

$$\Psi_{2,2} = \mathcal{A}\{\psi(12; 34)s_{10}t_6\} \quad (\text{E1})$$

Here,  $\mathcal{A}$  is an antisymmetrizer, and  $\psi(12; 34)$  is the spatial part of the deuteron wavefunctions. This wavefunction can be taken to be of the form

$$\psi(12; 34) = \phi_d(\mathbf{r}_2 - \mathbf{r}_1) \phi_d(\mathbf{r}_4 - \mathbf{r}_3) F_{2,2} \left( \frac{\mathbf{r}_1 + \mathbf{r}_2}{2}, \frac{\mathbf{r}_3 + \mathbf{r}_4}{2} \right) \quad (\text{E2})$$

There are two kinds of  $3 + 1$  wavefunctions, including singlet and triplet states. The singlet  $S = 0$  states can be written as

$$\Psi_{3,1} = \mathcal{A} \left\{ \psi(123; 4) \frac{1}{2} (s_5 t_6 - s_6 t_5) \right\} \quad (\text{E3})$$

The  $3+1$  triplet  $S = 1$  states can be written as

$$\Psi'_{3,1} = \mathcal{A} \left\{ \psi(123; 4) \frac{1}{2} (s_8 t_6 - s_9 t_5) \right\} \quad (\text{E4})$$

The spatial part of  $\Psi_{3,1}$  and  $\Psi'_{3,1}$  is of the form

$$\psi(123;4) = \phi_{3He}(\mathbf{r}_3 - \mathbf{r}_2, \mathbf{r}_2 - \mathbf{r}_1) F_{3,1} \left( \frac{\mathbf{r}_1 + \mathbf{r}_2 + \mathbf{r}_3}{3}, \mathbf{r}_4 \right) \quad (\text{E5})$$

## 2. Physical wavefunctions in terms of Yamanouchi basis states

All the physical wavefunctions for the initial and final states can be expressed as linear combinations of the Yamanouchi functions  $\Psi_1$ ,  $\Psi_4$  and  $\Psi_6$ . This is so because of group theoretical considerations and our assumptions that the spatial part of the deuteron, triton and helium wavefunctions are symmetric under the exchange of any two particles. The results in particular are

$$\Psi_{2,2} = \Psi_6 \quad (\text{E6})$$

with

$$\psi_5 = \frac{1}{\sqrt{12}} [2\psi(12;34) + 2\psi(34;21) - \psi(23;14) - \psi(14;23) - \psi(13;24) - \psi(24;13)] \quad (\text{E7})$$

$$\psi_6 = \frac{1}{2} [-\psi(23;14) - \psi(14;23) + \psi(13;24) + \psi(24;13)] \quad (\text{E8})$$

In the case of the singlet 3+1 channel, the antisymmetrizer acts to produce a single Yamanouchi basis state

$$\Psi_{3,1} = \Psi_1 \quad (\text{E9})$$

where the associated fully symmetric spatial part  $\psi_{10}$  can be expressed as

$$\psi_{10} = \frac{1}{2} [\psi(123;4) + \psi(124;3) + \psi(134;2) + \psi(234;1)] \quad (\text{E10})$$

In the case of the triplet 3+1 channel, the antisymmetrizer acts to produce a single Yamanouchi basis state

$$\Psi'_{3,1} = \Psi_4 \quad (\text{E11})$$

where the associated mixed symmetry spatial parts  $\psi_7$ ,  $\psi_8$ , and  $\psi_9$  are

$$\psi_7 = \frac{1}{\sqrt{12}} [3\psi(123;4) - \psi(124;3) - \psi(134;2) - \psi(234;1)] \quad (\text{E12})$$

$$\psi_8 = \frac{1}{\sqrt{6}} [2\psi(124;3) - \psi(134;2) - \psi(234;1)] \quad (\text{E13})$$

$$\psi_9 = \frac{1}{\sqrt{2}} [\psi(134;2) - \psi(234;1)] \quad (\text{E14})$$



## APPENDIX F: LATTICE CASE ANTISYMMETRIZATION

In this appendix we consider a partial antisymmetrization in the case of lattice wavefunctions. We retain the basic vacuum description for the four nucleons of the vacuum case, and extend the description to include the other nuclei as spectators.

### 1. Physical Wavefunctions

We can implement this program in the case of the initial states to write

$$\Psi_{2,2}^L = \mathcal{A}\{\psi(12;34, \{\mathbf{R}\})_{s_{10}t_6}\} \quad (\text{F1})$$

Here,  $\mathcal{A}$  is the antisymmetrizer acting on particles 1, 2, 3 and 4 only, and  $\psi(12;34, \{\mathbf{R}\})$  is the spatial part of the deuteron and the lattice wavefunctions. This wavefunction can be taken to be of the form

$$\psi(12;34) = \phi_d(\mathbf{r}_2 - \mathbf{r}_1) \phi_d(\mathbf{r}_4 - \mathbf{r}_3) F_{2,2}^L \left( \frac{\mathbf{r}_1 + \mathbf{r}_2}{2}, \frac{\mathbf{r}_3 + \mathbf{r}_4}{2}, \{\mathbf{R}\} \right) \quad (\text{F2})$$

There are two kinds of 3 + 1 wavefunctions, including singlet and triplet states. The singlet  $S = 0$  states can be written as

$$\Psi_{3,1}^L = \mathcal{A} \left\{ \psi(123;4, \{\mathbf{R}\}) \frac{1}{2} (s_5 t_6 - s_6 t_5) \right\} \quad (\text{F3})$$

The 3+1 triplet  $S = 1$  states can be written as

$$\Psi_{3,1}'^L = \mathcal{A} \left\{ \psi(123;4, \{\mathbf{R}\}) \frac{1}{2} (s_8 t_6 - s_9 t_5) \right\} \quad (\text{F4})$$

The spatial part of  $\Psi_{3,1}^L$  and  $\Psi_{3,1}'^L$  is of the form

$$\psi(123;4, \{\mathbf{R}\}) = \phi_{3He}(\mathbf{r}_3 - \mathbf{r}_2, \mathbf{r}_2 - \mathbf{r}_1) F_{3,1}^L \left( \frac{\mathbf{r}_1 + \mathbf{r}_2 + \mathbf{r}_3}{3}, \mathbf{r}_4, \{\mathbf{R}\} \right) \quad (\text{F5})$$

### 2. Physical wavefunctions in terms of Yamanouchi basis states

Now since our antisymmetrizer, acts only on the nuclear coordinates, and not on the  $\{\mathbf{R}\}$ , we see that the results of the vacuum case hold except that the spatial parts of the wavefunctions get augmented. For example, we may write

$$\Psi_{2,2}^L = \Psi_6 \quad (\text{F6})$$

with

$$\psi_5 = \frac{1}{\sqrt{12}} [2\psi(12; 34, \{\mathbf{R}\}) + 2\psi(34; 21, \{\mathbf{R}\}) - \psi(23; 14, \{\mathbf{R}\}) - \psi(14; 23, \{\mathbf{R}\}) - \quad (F7)$$

$$\psi(13; 24, \{\mathbf{R}\}) - \psi(24; 13, \{\mathbf{R}\})] \quad (F8)$$

$$\psi_6 = \frac{1}{2} [-\psi(23; 14, \{\mathbf{R}\}) - \psi(14; 23, \{\mathbf{R}\}) + \psi(13; 24, \{\mathbf{R}\}) + \psi(24; 13, \{\mathbf{R}\})] \quad (F9)$$

In the case of the singlet 3+1 channel, we obtain a similar connection to the Yamanouchi basis as in the vacuum case

$$\Psi_{3,1}^L = \Psi_1 \quad (F10)$$

where the spatial part is now augmented to include the spectator nuclei

$$\psi_{10} = \frac{1}{2} [\psi(123; 4, \{\mathbf{R}\}) + \psi(124; 3, \{\mathbf{R}\}) + \psi(134; 2, \{\mathbf{R}\}) + \psi(234; 1, \{\mathbf{R}\})] \quad (F11)$$

The triplet 3+1 channel becomes

$$\Psi_{3,1}'^L = \Psi_4 \quad (F12)$$

where

$$\psi_7 = \frac{1}{\sqrt{12}} [3\psi(123; 4, \{\mathbf{R}\}) - \psi(124; 3, \{\mathbf{R}\}) - \psi(134; 2, \{\mathbf{R}\}) - \psi(234; 1, \{\mathbf{R}\})] \quad (F13)$$

$$\psi_8 = \frac{1}{\sqrt{6}} [2\psi(124; 3, \{\mathbf{R}\}) - \psi(134; 2, \{\mathbf{R}\}) - \psi(234; 1, \{\mathbf{R}\})] \quad (F14)$$

$$\psi_9 = \frac{1}{\sqrt{2}} [\psi(134; 2, \{\mathbf{R}\}) - \psi(234; 1, \{\mathbf{R}\})] \quad (F15)$$

## APPENDIX G: INTEGRALS RESULTING FROM PERMUTATIONS

Due to the antisymmetrization, we generate a total of twenty four terms in the matrix element example in the main body of the paper. These are

$$\begin{aligned}
\sqrt{12} \langle \Psi_{3,1}(M_s = 0) | V(1, 2) | \Psi_{2,2}(M_s = 1) \rangle = & \\
& \int \psi(123; 4)^* v(1, 2) \psi(12; 34) + \int \psi(123; 4)^* [v(1, 2) - \frac{1}{2}v(1, 4) - \frac{1}{2}v(4, 1)] \psi(12; 43) \\
& + \int \psi(123; 4)^* [v(1, 4) - v(1, 2)] \psi(14; 23) + \int \psi(123; 4)^* v(4, 1) \psi(41; 23) + \int \psi(123; 4)^* v(1, 2) \psi(34; 12) \\
& + \int \psi(123; 4)^* [v(1, 2) - \frac{1}{2}v(1, 4) - \frac{1}{2}v(4, 1)] \psi(43; 12) + \int \psi(123; 4)^* [-v(1, 2) + v(1, 4)] \psi(23; 14) \\
& + \int \psi(123; 4)^* v(4, 1) \psi(23; 41) + \int \psi(123; 4)^* [-v(1, 2)] \psi(24; 13) \\
& + \int \psi(123; 4)^* [-\frac{1}{2}v(1, 4) - \frac{1}{2}v(4, 1)] \psi(42; 13) + \int \psi(123; 4)^* [-v(1, 2)] \psi(13; 24) \\
& + \int \psi(123; 4)^* [-\frac{1}{2}v(1, 4) - \frac{1}{2}v(4, 1)] \psi(13; 42) \tag{G1}
\end{aligned}$$

where  $V(1, 2)$  is some general nuclear potential which contains spin and isospin dependent terms, and where  $v(i, j)$  is the spatial interaction between particles  $i$  and  $j$  which is obtained by carrying out the spin and isospin algebra. In the special case that  $V(1, 2) = V_{HJ}(1, 2)$ , then  $v(i, j) = V_R^{10,5}(i, j)$ .

Some of these terms are amenable to a simple interpretation in terms of stripping reactions. Others can be considered as higher-order exchange terms. However, in nuclear reactions, it is not necessary that higher order exchange terms are necessarily less important than simple direct or exchange interactions. Hence, in any realistic computation we will need to sum over all of these terms.

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